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A PHYSICALLY BASED MODEL FOR INTERPRETING THE ELECTROCATALYTIC ACTIVITY OF NANOPARTICLES FOR SOLID OXIDE FUEL CELL ANODES

Daniel Drasbæk[1,a], Bhaskar Reddy Sudireddy[1], and Peter Holtappels[1]

[1]Department of Energy Conversion and Storage, Technical University of Denmark, Denmark,
[a]dadr@dtu.dk

Over the past decades, research in the solid oxide cells has gain tremendous momentum. However, characterizing the electrocatalytic activity of all solid-state materials is limited to a very few techniques due to the complexity of the placement of reference electrodes. One way of characterizing the electrocatalytic activity is to analyse the activation energy of the electrochemical reaction. Nonetheless, it can be misleading to look only at the activation energy, which in the end can lead to false conclusions, since the activation energy does not reflect the real performance of the cells, but has to be coupled to other electrochemical results, like the polarization resistance, the pre-exponential factor, etc.
During the screening for new electrocatalyst nanoparticles for the solid oxide fuel cell electrodes, it was found that the interpretation of the data was not as direct as first anticipated. It was necessary to develop a physically based model that could describe the changes observed in both the activation energy and the pre-exponential factor of the electrochemical reaction, when the atmosphere was changed.
This work propose a model, which is based on the simple harmonic oscillator, were the metal nanoparticle interacts with the adsorbed reactant in accordance to Hooke's law. By interpreting the activation energy as the binding energy of the adsorbed species and thereby as the force between the adsorbed species and the metal nanoparticles, one can correlate the changes seen in the activation energy, with the changes observed in the pre-exponential factor through the simple harmonic oscillator and Hooke's law. When the fuel atmosphere is changed from one to another, changes in the electrochemical reaction is observed. One is then, by using the presented model, able to distinguish between changes in the nature of reactants of the electrochemical reaction, e.g. through their mass, and changes in the kinetics e.g. the turnover frequency, of the electrochemical reaction. All of which can in the end be coupled with the overall polarization resistance of the reaction and hence give rise to a more realistic description of the electrocatalytic activity.